ISSN 0029-3865

CBPF-NF-040/89

A GENERALISED HUBBARD HAMILTONIAN: INFLUENCE OF TEMPERATURE AND FRACTALITY

by

Sérgio A. CANNAS*+, Francisco A. TAMARIT*+ and
Constantino TSALLIS*

*Centro Brasileiro de Pesquisas Físicas - CBPF/CNPq
Rua Dr. Xavier Sigaud, 150
22290 - Rio de Janeiro, RJ - Brasil

+Facultad de Matemática, Astronomia y Física/UNC
Laprida 854, 5000-Córdoba, Argentina

ABSTRACT

We consider a generalised Hubbard Hamiltonian which is invariant under a Real Space Renormalisation Group. Within the present approximation, the Bravais lattice is replaced by a diamond-like hierarchical lattice. We calculate the phase diagram associated with the half-filled band Hubbard Hamiltonian in d = 1, 2 and 3, in the full range of the dimensionless intra-atomic interaction U and hopping t parameters. The influence of the hierarchical lattice fractality is analised as well.

KEYWORDS : Hubbard model, real space renormalisation group, hierarchical lattice.

PACS index : 05.30, 71.90, 71.45.

The Hubbard Hamiltonian [1] (hereafter denoted by H) provides the most simple model to study the correlation effects of electrons in narrow energy bands, like metallic magnetism [2] and the metal-insulator transition [3,4] (Mott transition). Moreover, in the last years there was an increasing interest in this model because of its applications in the study of high Tc oxide superconductors [5-12].

The dimensionless Hubbard Hamiltonian $\mathcal{H}_H$ is defined as

$$\mathcal{H}_H \equiv -\beta(H-\mu' N) = t \sum_{\langle i,j\rangle,\sigma} (c^+_{i\sigma} c_{j\sigma} + c^+_{j\sigma} c_{i\sigma}) - U \sum_i n_{i\uparrow} n_{i\downarrow} + \mu \sum_{i,\sigma} n_{i\sigma} \quad (1)$$

where $\beta \equiv 1/k_B T$, $c^+_{i\sigma}(c_{i\sigma})$ is the creation (annihilation) operator for an electron with spin $\sigma = \pm 1$ in a Wannier state centered at the site i of the lattice, $n_{i\sigma} \equiv c^+_{i\sigma} c_{i\sigma}$ is the corresponding occupation number, and μ' is the chemical potential. We shall consider the half-filled band case, which implies $\mu = U/2$. We can then rewrite the Hamiltonian (1) as

$$\mathcal{H}_H = t \sum_{\langle i,j\rangle,\sigma} (c^+_{i\sigma} c_{j\sigma} + c^+_{j\sigma} c_{i\sigma}) + U/2 \sum_i (n_{i\uparrow} - n_{i\downarrow})^2 \quad (2)$$

In order to study the thermodynamics of the Hubbard model, at least as far as criticality is concerned, we use a Real Space correlation-function-preserving Renormalisation Group (RG) method. Our approximation consists in replacing the Bravais lattices by diamond-like hierachical lattices, namely those associated with the clusters shown in Fig.1. In order to obtain the RG recurrence equations, a decimation-like procedure is carried out over the degrees of freedom associated with the internal sites of the clusters. This method proved to be an useful one in a variety of quantum magnetic systems (e.g., anisotropic spin 1/2 Heisenberg model [14,15]).

The recurrence equations are obtained by imposing

$$\exp(\mathcal{H}' + \mathbb{C}) = \operatorname{Tr}_{\text{internal sites}} \exp(\mathcal{H}) \quad (3)$$

where $\mathcal{H}$ denotes the Hamiltonian associated with the cluster, $\mathcal{H}'$ denotes the renormalised Hamiltonian of the two-sites chain and the partial trace operation is carried out by summing over the set of occupation numbers associated with the internal sites of the cluster.

In particular, Hamiltonian (2) does not satisfy relation (3). Therefore we have to search for a generalization of the Hubbard Hamiltonian (2) which might satisfy this relation.

This generalised Hamiltonian can be obtained without explicitly carring out the decimation procedure, by using the symmetries of the Hamiltonian (2) that are preserved by (3).

As usually, we define the spin and charge operators as

$$\begin{aligned} S_i^z &= n_{i\uparrow} - n_{i\downarrow} & \rho_i^z &= n_{i\uparrow} + n_{i\downarrow} - 1 \\ S_i^- &= C_{i\downarrow}^+ C_{i\uparrow} & \rho_i^- &= C_{i\downarrow} C_{i\uparrow} \\ S_i^+ &= C_i^+ C_{i\downarrow} & \rho_i^+ &= C_i^+ C_{i\downarrow}^+ \end{aligned} \qquad (4)$$

The fermionic character of the C's operators imposes the following relations

$$\left(S_i^{\nu} \right)^2 + \left(\rho_i^{\nu'} \right)^2 = 1$$

$$S_i^{\nu} \rho_i^{\nu'} = 0 \qquad \nu, \nu' = x, y, z$$

where

$$\begin{aligned} S_i^x &= S_i^+ + S_i^- & \rho_i^x &= \rho_i^+ + \rho_i^- \\ S_i^y &= -i(S_i^+ - S_i^-) & \rho_i^y &= -i(\rho_i^+ - \rho_i^-) \end{aligned} \qquad (5)$$

We now introduce a unitary transformation U_ρ, defined as (see reference [16]).

$$U_\rho = \prod_i \exp\left(i\gamma_i \vec{q}_i . \vec{\rho}_i \right) \qquad (6)$$

where the $\{\vec{q}_i\}$ are arbitrary unit vectors and the $\{\gamma_i\}$ are the

parameters of the transformation. If $\vec{q}_i = \vec{q}$ for every site i, and $\vec{q}$ lies in the x-y plane, this transformation generalises the particle-hole exchange transformation.

The symmetries of (2) that are preserved under (3) are the following ones :

(a) rotational invariance ($\mathcal{H}_H$ commutes with $\vec{S} \equiv \Sigma_i \vec{S}_i$);
(b) invariance under U_ρ when $\vec{q}_i = \vec{q}$ is in the z direction and $\gamma_i = \gamma$ for all sites i. In this case U_ρ corresponds to a trivial phase change of the Wannier representation ($\varphi_i(x) \longrightarrow e^{\gamma_i} \varphi_i(x)$, $\varphi_i(x)$ being the Wannier orbital located at site i).
(c) invariance under U_ρ when $\vec{q}_i = \vec{q}$ lies in the x-y plane provided that we choose $\gamma_i = -\gamma_j$, with i,j being nearest-neighboring sites. Such a choice is not always possible (e.g. frustrated clusters), therefore the choice of the cluster must be careful in order to apply the present method.

For simplicity let us first analise the 1-d case. In one dimension the smallest cluster which preserves the symmetry (c) is a four-site chain (see Fig. 1-a). Indeed, if a three-site chain was used, then the Hamiltonian resulting from $\mathcal{H}_H$ through (3), i.e. by taking the parcial trace over the internal site, would not be invariant under (c); it would rather be invariant under U_ρ with $\vec{q}$ in the x-y plane and $\gamma_i = \gamma$ for all i. This Hamiltonian clearly will not contain the original Hubbard Hamiltonian as a particular case [16,17] . If the four-site chain is instead used, the partial trace in (2) over the two internal sites will leave the desired generalised Hamiltonian which satisfies all our requirements. To be more explicit, if we atribute alternating $+\gamma$ and $-\gamma$ to each site of the chain, the four-site chain leaves, under decimation $\gamma_1 = +\gamma$ and $\gamma_2 = -\gamma$ for the two-site chain, while the three-site chain leaves $\gamma_1 = \gamma_2 = +\gamma$.

We are now able to generalize the half-filled band Hubbard Hamiltonian. We consider all the one- and two-site operators which are invariant under the three symmetries mentioned above. A linear

combination of such terms yields the desired Hamiltonian, namely

$$\mathcal{H}_a = -J\sum_{<i,j>}\vec{S}_i.\vec{S}_j - K\sum_{<i,j>}(S_i^z)^2(S_j^z)^2 + U/2\sum_i (S_i^z)^2 -$$

$$-I\sum_{<i,j>}[\rho_i^z\rho_j^z - (\rho_i^x\rho_j^x + \rho_i^y\rho_j^y)] + t\sum_{<i,j>\sigma}(C_{i\sigma}^+C_{j\sigma} + C_{j\sigma}^+C_{i\sigma}) +$$

$$+D\sum_{<i,j>\sigma}(C_{i\sigma}^+C_{j\sigma} + C_{i\sigma}^+C_{j\sigma})(n_{i-\sigma} - n_{j-\sigma})^2 \qquad (7)$$

This is the minimal Hamiltonian which satisfies (3) and contains (2) as a particular case.

We note the following properties :

i) For J = K = I = D = 0 we recover the half-filled band Hubbard Hamiltonian (2), as expected.

ii) For t = D = I = 0 the Hamiltonian (7) leads to a quantum analog of the BEG (Blume-Emery-Griffiths) Hamiltonian.

iii) Using transformation (6) it can be shown that the grand partition function asociated with (7) satisfies $\mathcal{Z}(t,D) = \mathcal{Z}(-t,-D)$.

iv) Using transformation (6) it can be shown that Hamiltonian (7) preserves the half-filled band character of (2).

The above arguments not only apply to a linear chain, but to all two-terminal clusters whose topology enables them to satisfy the invariance property (c).

The generalised Hamiltonian $\mathcal{H}_a$ being now constructed, the recurrence equations between the parameters of $\mathcal{H}_a$ and $\mathcal{H}_a'$ can be obtained by explicitly computing the partial trace (3). These relations cannot be obtained analytically, since the calculation of $\exp(\mathcal{H}_a)$ involves the diagonalization of very large matrices; consequently part of the calculations were done numerically.

We analised the RG flow of points in the parameter space (J,I,K,U,t,D) for d = 1, 2 and 3. Then we obtained the section of this complex phase diagram with the (U,t) plane

(i.e. I = J = K = D = 0) for both signs of U.

In d = 1 there is no phase transition for any value of U ≠ 0 as expected [18]. For U/t > 0 the system is an insulator, for U/t = 0 it is a normal metal and for U/t < 0 it is in a metallic phase characterised by uncorrelated pairs of electrons.

In d = 2 we find the same structure as in d = 1. All points in the U/t = 0 axis with 1/t ≠ 0 are attracted by the fixed point (U/t,1/t,I,J,K,D) = (0,∞,0,0,0,0), which charaterises a normal metallic phase. There are two fully stable fixed points, namely (U/t,1/t,I,J,K,D) = (± ∞,∞,0,0,0,0). All points with U/t > 0 and 1/t ≠ 0 are attracted by the fixed point (+∞,∞,0,0,0,0), while points with U/t < 0 and 1/t ≠ 0 are attracted by (−∞,∞,0,0,0,0). In the limit U/t → ∞ the Hubbard model is asymptotically equivalent to an antiferromagnetic Heisenberg model, therefore we can conclude that for U/t >0 and 1/t ≠ 0 the system is a paramagnetic insulator. There is no Mott transition for finite U/t in the ground state (i.e., 1/t = 0). This results are in agreement with previous ones obtained by a different RG technique [19], and by Monte Carlo calculations [20] . In the limit U/t → −∞ the Hubbard model is asymptotically equivalent to a gas of bosons with hard cores and long-ranged interactions. These bosons are bound pairs of electrons. However for d = 2 there is neither superconductivity nor charge density waves for finite temperature. Therefore for U/t < 0 and 1/t ≠ 0 the system is in a metallic phase characterised by uncorrelated pairs of electrons without any magnetic order [22].

For d = 3 the calculated phase diagram is shown in Fig.2. For U/t > 0 the system is always an insulator and there is a second order phase transition from a paramagnetic state to an antiferromagnetic state. For U/t < 0 there is a second order phase transition from a phase characterised by uncorrelated pairs of electrons at high temperature to a mixed phase characterised by charge density waves (CDW) and singlet superconductivity (SS) at low temperature, both without magnetic order [13]. The two

critical lines for $U/t > 0$ and $U/t < 0$ join at a point $1/t_c \neq 0$ in the $U/t = 0$ axis (pure tight-binding limit). For $U/t = 0$ and $1/t > 1/t_c$ all the points are attracted by the $1/t = \infty$ fixed point, that is, that region corresponds to a metallic phase. For $1/t < 1/t_c$ we found an anomalous behavior in the renormalisation flow. All the points are attracted by limit cycles of order two rather than being attracted by normal fixed points. More precisely, the points are attracted by one or the other of two different cycles characterised as indicated in table I. The basins of attraction of these two cycles appear alternatively along the $U/t = 0$ axis for $0 < 1/t < 1/t_c$. We believe that this behavior is owed to the fractality of the lattice that has been used. It is known that tight-binding systems present many peculiar properties when defined on fractal lattices : fractal spectrum, localised states, hierarchal states [21] and other anomalies (see Fig. 1 of Ref. [24]). Therefore any operation involving rescaling (Eq. 3) will be strongly affected when Bravais lattices are replaced by fractal ones, as in our case. At the time, it is not clear the physical meaning (if any) of these fixed cycles. Note that the two cycles are related by the transformation $t \rightarrow -t$, $0 \rightarrow -0$, so it is clear that these two cycles in fact represent essentially the same physical state, since the grand partition function remains invariant under this transformation. Concerning the shape of the critical line, for say $U/t > 0$, one expects, for a Bravais lattice, the existence of a maximum for $U/t \neq 0$ [23]. This is not observed in the present calculation, possibly due to the fractality of the lattice.

It is also worthy to stress that no Mott transition is observed at vanishing temperature and $U/t \neq 0$. In fact we think that the localising effect associated with the fractal character of the lattice is strong enough to destroy such possibility.

In Fig.3 we show t_c as a function of the dimension d. We observe a critical dimension $d_c \cong 2.41$. In addition to that, we find the same value for the lower critical dimension of the para-antiferromagnetic transition for $U/t \gg 1$. This suggests that the whole critical line disappears for $d = d_c$.

Let us focus the case of non half-filled band.In this case Hamiltonian (1) loses symmetry (c), and we obtain that the Hamiltonian which generalises (1) and remains invariant under (3) is the following one :

$$H_a = - J \sum_{<i,j>} \vec{S}_i . \vec{S}_j - K \sum_{<i,j>} (S_i^z)^2 (S_j^z)^2 - U \sum_i n_{i\uparrow} n_{i\downarrow} + \mu \sum_{i\sigma} n_{i\sigma}$$

$$- I_2 \sum_{<i,j>} \rho_i^z \rho_j^z + I_1 \sum_{<i,j>} (\rho_i^x \rho_j^x + \rho_i^y \rho_j^y) + t \sum_{<i,j>\sigma} (C_{i\sigma}^+ C_{j\sigma} + C_{j\sigma}^+ C_{i\sigma})$$

$$+ D_1 \sum_{<i,j>\sigma} (C_{i\sigma}^+ C_{j\sigma} + C_{i\sigma}^+ C_{j\sigma}) (n_{i-\sigma} + n_{j-\sigma})$$

$$- 2D_2 \sum_{<i,j>\sigma} (C_{i\sigma}^+ C_{j\sigma} + C_{i\sigma}^+ C_{j\sigma}) n_{i-\sigma} n_{j-\sigma} \qquad (8)$$

The phase diagram associated with this hamiltonian is under study and will be published elsewhere.

In summary, the present approach shows to be a powerfull one to study critical propierties of a great variety of fermionic systems related to the Hubbard model, since the generalised Hamiltonian (8) explicitly contains terms which account for charge fluctuations, magnetic order and hopping. In particular we have seen that for d = 2 the fractality of the lattice does not affect, at least qualitatively, the phase diagram associated with the half-filled band Hubbard Model for Bravais lattices. In view of these results, we think that this approach can provide a new method to study high T_c superconductivity in CuO compounds by considering the non-half-filled band case, since (8) contains many of the basic interactions that have been proposed to explain this phenomenon [5-11].

In the d = 3 case the present approach does not exhibit the metal-insulator transition which is expected in Bravais lattices. In spite of that, it provides an interesting method to analise the interplay between correlations and fractality in fermionic systems

in the weak correlation limit $U/t \ll 1$. Moreover, in the strong correlation limit $U/t \gg 1$, the fractality seems to have a negligeable influence on the phase diagram. Consequently we expect our model to be an useful one for studyng superconductivity also in the same limit ($U/t \gg 1$). Work along these lines is in progress.

We wish to thank D. Prato, E. M. F. Curado, R. Maynard and L. M. Falicov for fruitful discussions and suggestions. Two of us (S.A.C. and F.A.T) thanks CNPq (Brazil) for financial support.

Captions for figures and tables

Fig. 1 : Renormalisation group-cell transformation. $\bar{L}$ stands for the set of parameters (U, K, J, I, D, t). a) d = 1; b) d = 2; c) d = 3.

Fig. 2 : Phase diagram of the half-filled Hubbard model in d = 3 in a hierarchical lattice (1/t ≡ dimensionless temperature).

Fig 3 : $1/t_c$ vs. the intrinsic dimensionality d of the hierarchical lattice.

Table I : Limit cycles for U/t = 0 and $1/t < 1/t_c$. The parameters (U, K, J, I, t) have fixed values while the parameter D oscillates between the values $D^{(1)}$ and $D^{(2)}$.

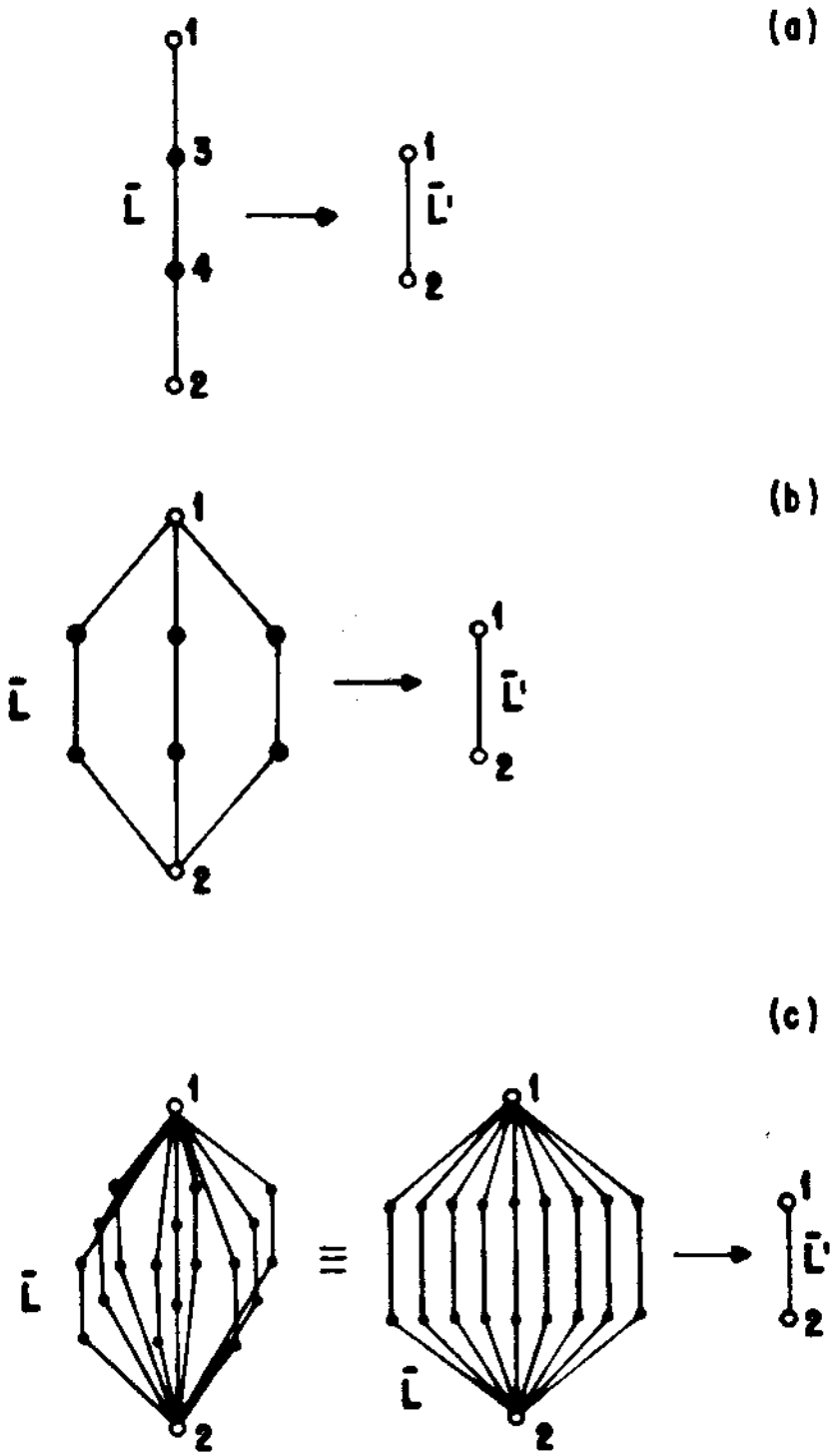

FIG.1

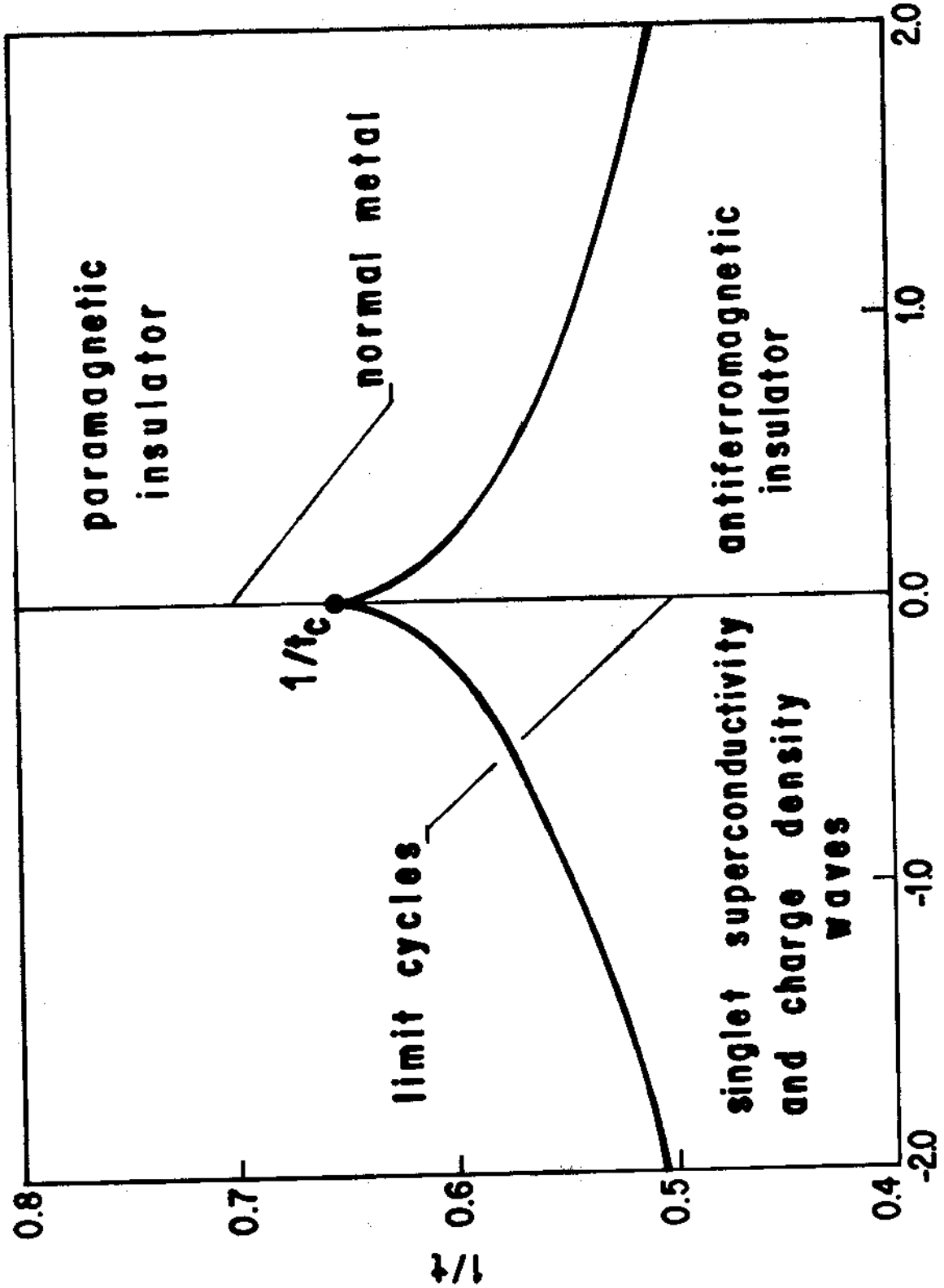
paramagnetic
insulator
normal metal
antiferromagnetic
insulator
1/t_c
limit cycles
singlet superconductivity
and charge density
waves
0.8
0.7
0.6
0.5
0.4
1/t
2.0
1.0
0.0
-1.0
-2.0
U/t

FIG.2

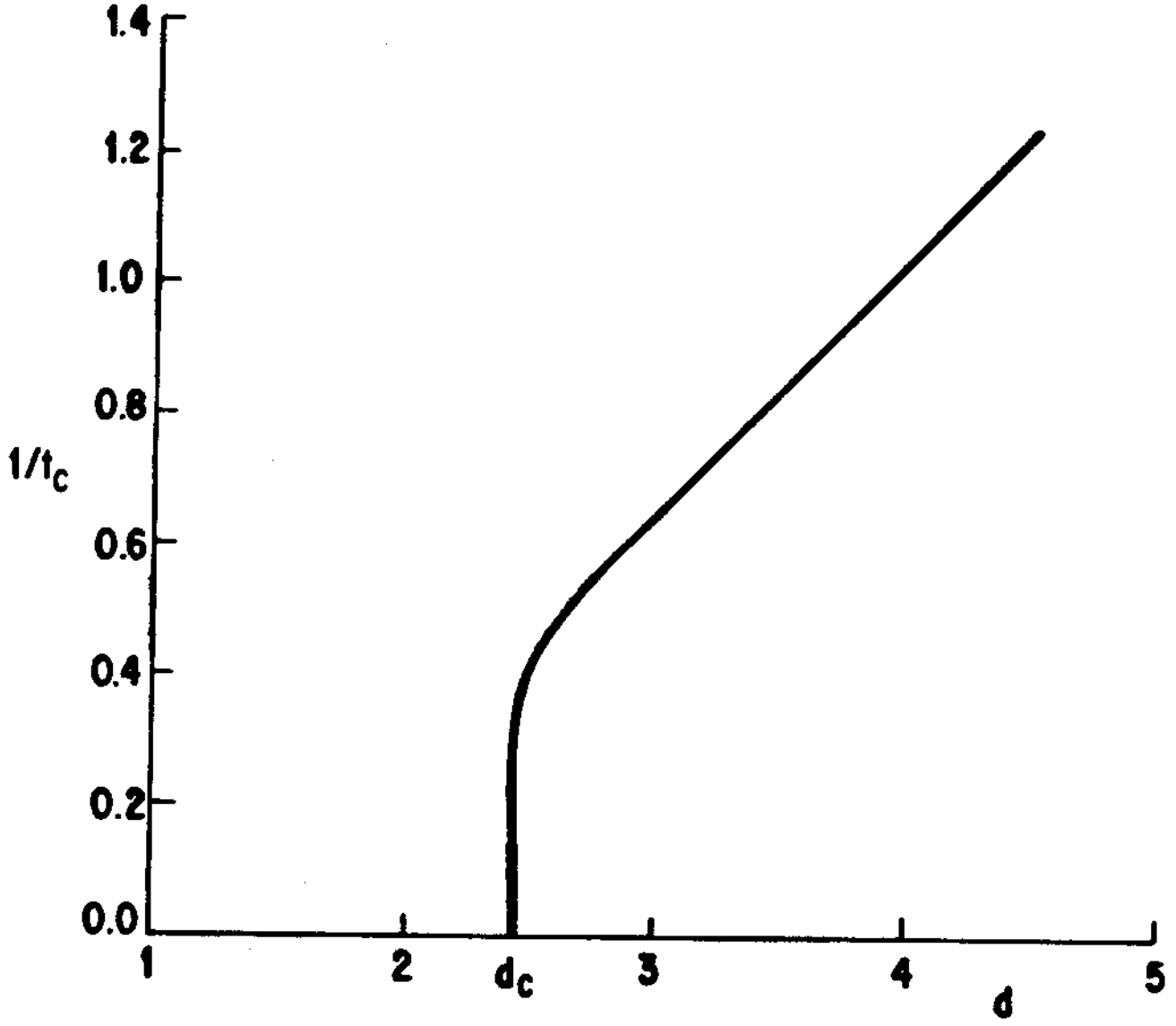

FIG. 3

cycle	U	K	I	J	t	$D^{(1)}$	$D^{(2)}$
A	1.406	0.703	0.07	0.07	7.513	0.607	-15.63
B	1.406	0.703	0.07	0.07	-7.513	-0.607	15.63

Table I

REFERENCES

[1]. J. Hubbard, Proc. R. Soc. A 276, 238 (1963).

[2]. Y Nagaoka, Phys. Rev. 147, 392 (1966).

[3]. W. F. Brinkman and T. M. Rice, Phys. Rev. B 2,4302 (1970).

[4]. M. Cyrot, J. Physique 33, 125 (1972).

[5]. P. W. Anderson, Science 235, 1196 (1987).

[6]. V. J. Emery, Phys. Rev. Lett. 58, 2794 (1987).

[7]. M. Cyrot, Solid State Commun. 62, 821 (1987); 63, 1015 (1987).

[8]. C. R. Proetto and L. M. Falicov, Phys. Rev. B 15, 1754 (1988).

[9]. J.R. Schrieffer, X.G. Wen and S.C, Zhang, Phys. Rev. Lett. 60, 944 (1988).

[10]. Wei-ming Que and G. Kirczenow, Z. Phys. B 73, 425 (1989).

[11]. B. I. Shraiman and E. D. Siggia, Phys. Rev. Lett. 60, 740 (1988).

[12]. R. Micnas, J. Ranninger and S. Robaszkiewicz, J. Phys. C 21, L145 (1988).

[13]. S. Robaszkiewicz, R. Micnas and K. A. Chao, Phys. Rev. B 23, 1447 (1981).

[14]. A. O. Caride, C. Tsallis and S. I. Zanette, Phys. Rev. Lett. 51, 145 (1983); 51, 616 (1983).

[15]. A. M. Mariz, C. Tsallis and A. O. Caride, J. Phys. C 18, 4189 (1985).

[16]. C. Castellani, C. DiCastro, D. Feinberg and J. Ranninger, Phys. Rev. Lett 43, 1957 (1979).

[17]. H. Takano and M. Suzuki, Physica 109A, 618 (1981),

[18]. E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. 20, 1445 (1968).

[19]. C. Vanderzande, J. Phys. A 18, 889 (1985).

[20]. J. Hirsch, Phys. Rev. Lett. 51, 1900 (1983).

[21]. R. Rammal, J. Physique 45, 191 (1984).

[22]. V.J. Emery, Phys. Rev. B 14,2989 (1976).

[23]. R.R. DeMarco, E.N. Economou and C.T. White, Phys. Rev. B 18, 3968 (1978).

[24]. C. Tsallis and R. Maynard, Phlys. Lett. A 129, 118 (1988).